

Anomalous thermal conductivity and local temperature distribution on harmonic Fibonacci chains

Masashi Torikai and Takashi Odagaki

Department of Physics, Kyushu University, Fukuoka 812-8581

Abstract. The harmonic Fibonacci chain, which is one of a quasiperiodic chain constructed with a recursion relation, has a singular continuous frequency-spectrum and critical eigenstates. The validity of the Fourier law is examined for the harmonic Fibonacci chain with stochastic heat baths at both ends by investigating the system size N dependence of the heat current J and the local temperature distribution. It is shown that J depends on N as $J \sim (\ln N)^{-1}$ and the local temperature strongly oscillates along the chain. These results indicate that the Fourier law does not hold on the harmonic Fibonacci chain. Furthermore the local temperature exhibits two different distribution according to the generation of the Fibonacci chain, i.e., the local temperature distribution does not have a definite form in the thermodynamic limit. The relations between N -dependence of J and the frequency-spectrum, and between the local temperature and critical eigenstates are discussed.

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Many studies in these decades have shown that arbitrarily defined one-dimensional (1D) systems of interacting particles do not exhibit normal thermal transport properties, i.e., the Fourier law does not hold on such systems [1, 2, 3, 4, 5]. For the steady-state of the homogeneous 1D chain of system size N , the Fourier law, $J = -\kappa \nabla T$ with thermal conductivity κ , indicates that the heat current depends on the system size as $J \sim 1/N$ and that the temperature gradient ∇T is constant along the chain. Rieder *et al* [1] have shown for a 1D chain of equal mass particles interacting with identical harmonic potential that the heat current is independent of the system size. They also have obtained the local temperature distribution. The local temperature behaves in unphysical way: the temperature takes a constant value in the bulk. Furthermore, near the end of the chain, the temperature decreases as we move in the direction of the hotter heat bath, and rise only at the end particle in contact with the heat bath; the temperature exhibits corresponding behavior at the other end of the chain. Casher and Lebowitz [2] have shown for the same model but with random mass distribution that $J \sim N^{-3/2}$. For the same random mass distribution model but with different type of boundary conditions, Rubin and Greer [3] have obtained the result $J \sim N^{-1/2}$. These system size dependence of J for periodic or disordered chains may be attributed to the localization property of eigenstates on these chains. Since the eigenstates are extended in periodic chains, the ballistic energy transport of extended eigenstates results in the constant heat current of the periodic chains.

In contrast, for the disordered chains, the decrease in heat current with increasing system size is caused from the localized eigenstates, which can not transport energy over the length of the system. The extended and localized eigenstates correspond to continuous and pure-point spectra, respectively. It is shown that, for the Casner and Lebowitz type chain and heat bath, the thermal conductivity κ diverges as the system size increases if the spectrum contains absolutely continuous part [2].

Some of quasiperiodic systems have a Cantor set-like spectrum, i.e., a singular continuous spectrum [6, 7, 8, 9, 10]. Then, on such systems, eigenstates show power law decay; such neither extended nor exponentially localized states are called critical states [6]. For example, a harmonic chain with quasiperiodically arranged spring constants and/or mass of particles has a singular continuous spectrum and critical eigenstates [7, 8, 9]. We may thus expect that such quasiperiodic systems show exotic heat transport properties compared with periodic or disordered systems.

In the present paper we investigate the anomaly of heat transport phenomena on harmonic Fibonacci chains, which is one of discrete quasiperiodic and self-similar 1D lattices. We focus the anomaly resulting from the spectral properties of the Fibonacci chain. In order to check the validity of the Fourier law on the Fibonacci chain, we investigate the system size dependence of the heat current J . Although Maciá [11] have already studied the thermal conductivity κ of the harmonic Fibonacci chain, he has not checked the system size dependence of κ and thus the validity of the Fourier law is not clear yet. Our results show that the heat current behaves as $J \sim (\ln N)^{-1}$, which is in contrast with that of periodic or disordered chain. We discuss the fact that the total bandwidth of the phonon spectrum of the Fibonacci chain has similar N dependence to J . We also calculate the local temperature distribution on the Fibonacci chain; it seems not to converge to a definite form even in the thermodynamic limit. We relate $\{T_i\}$ with the critical eigenstates of the Fibonacci chain.

The harmonic Fibonacci chain which we consider is a 1D chain of N particles; each particle interact with its neighbouring particles with equal spring constant k . We make the sequence of mass of particles $\{m_i | i = 1, \dots, N, m_i = m_\alpha \text{ or } m_\beta\}$ according to the Fibonacci sequence. The Fibonacci sequence of the n -th generation L_n , which consists of two kinds of components m_α and m_β , is constructed by the recursion relation: $L_n = L_{n-1}L_{n-2}$, $L_0 = m_\beta$, and $L_1 = m_\alpha$. Then the system size of the n -th generation Fibonacci sequence is the Fibonacci number F_n , which obeys the recursion relation $F_n = F_{n-1} + F_{n-2}$, $F_0 = 1$, and $F_1 = 1$. The Fibonacci number F_n is asymptotically behaves as $F_n \sim \tau^n$ with golden ratio $\tau = (\sqrt{5} + 1)/2$. We can obtain the asymptotic properties of the Fibonacci chain in the limit of $N \rightarrow \infty$ by concerning the infinite-generation limit $n \rightarrow \infty$. We set both the spring constant k and the mass m_β unity; we calculate the heat current and the temperature distribution varying with the mass m_α .

We consider the following Langevin equations for particles of the chain with stochastic heat baths at both ends:

$$\begin{aligned} m_1 \ddot{x}_1 &= -2x_1 + x_2 - \gamma \dot{x}_1 + \eta_L(t), \\ m_i \ddot{x}_i &= -2x_i + x_{i-1} + x_{i+1}, \\ m_N \ddot{x}_N &= -2x_N + x_{N-1} - \gamma \dot{x}_N + \eta_R(t), \end{aligned} \tag{1}$$

where x_i are the displacements of the particles from their equilibrium positions; γ is the friction constant; η_L and η_R are the random forces caused from left and right heat baths, respectively. We choose the random forces the white noises, i.e., the Fourier

transforms of the random force obey

$$\begin{aligned}\langle \eta_L(\omega) \eta_L(\omega') \rangle &= 4\pi\gamma T_L \delta(\omega + \omega'), \\ \langle \eta_R(\omega) \eta_R(\omega') \rangle &= 4\pi\gamma T_R \delta(\omega + \omega'),\end{aligned}\quad (2)$$

where angular bracket is the average over the random force; T_L and T_R are the temperatures of the left and right heat baths, respectively.

The energy current J_i from the site i to the site $i + 1$ is

$$J_i = \frac{1}{2} \langle (\dot{x}_{i+1} + \dot{x}_i)(x_{i+1} - x_i) \rangle. \quad (3)$$

In the steady state, the energy current does not depend on the site; then from the Langevin equation (1),

$$J = \Delta T \int_0^\infty \frac{d\omega}{\pi} \frac{2\gamma^2 \omega^2}{|\det Y|^2}, \quad (4)$$

where $\Delta T = T_L - T_R$ and $Y = \Phi - \omega^2 M + i\gamma\Gamma$ with $\Phi_{ij} = -\delta_{i,j-1} + 2\delta_{ij} - \delta_{i,j+1}$, $M_{ij} = m_i \delta_{ij}$, and $\Gamma_{ij} = \gamma(\delta_{i,1} + \delta_{i,N})\delta_{i,j}$. We may write

$$\det Y = D_{1,N} - \gamma^2 \omega^2 D_{2,N-1} + i\gamma\omega(D_{2,N} + D_{1,N-1}), \quad (5)$$

where $D_{i,j}$ denotes the determinant of the sub-matrix of $\Phi - \omega^2 M$ which begins with i -th row and column and ends with j -th row and column [4].

We define the local temperature at site i

$$T_i = \left\langle p_i \frac{\partial H}{\partial p_i} \right\rangle = \left\langle \frac{p_i^2}{m_i} \right\rangle, \quad (6)$$

where H is the Hamiltonian of the system. We note that the equipartition relation $T_i = \langle x_i \partial H / \partial x_i \rangle$ holds for any mass distribution (for periodic case, the equipartition relation has proven in [1]). For our model we can write the explicit form of the local temperature as

$$T_i = T_L - m_i \gamma \Delta T \int_{-\infty}^\infty \frac{d\omega}{\pi} \cdot \omega^2 \left| \frac{D_{1,i-1} + i\gamma\omega D_{2,i-1}}{\det Y} \right|^2. \quad (7)$$

In calculating the heat current, it is convenient to express the determinant $D_{i,j}$ in terms of a transfer matrix as

$$\begin{pmatrix} D_{i,j} & -D_{i+1,j} \\ D_{i,j-1} & -D_{i+1,j-1} \end{pmatrix} = M_j M_{j-1} \cdots M_{i+1} M_i, \quad (8)$$

where the matrix $M_i(\omega)$ is the unimodular transfer matrix of site i defined as

$$M_i(\omega) = \begin{pmatrix} 2 - m_i \omega^2 & -1 \\ 1 & 0 \end{pmatrix}. \quad (9)$$

If we rewrite the total transfer matrices of the n -th generation Fibonacci chains as $\mathcal{M}_n = M_N M_{N-1} \cdots M_1$ with $N = F_n$, then \mathcal{M}_n obey a recursion relation

$$\mathcal{M}_n = \mathcal{M}_{n-2} \mathcal{M}_{n-1}, \quad \mathcal{M}_0 = \begin{pmatrix} 2 - m_\beta \omega^2 & -1 \\ 1 & 0 \end{pmatrix}, \quad \text{and} \quad \mathcal{M}_1 = M_1. \quad (10)$$

Since we can obtain all the determinants $D_{i,j}$ needed in (5) by calculating \mathcal{M}_n , the recursion relation (10) saves a lot of time in calculating J .

We calculated the heat current and the local temperature by numerical integration of (4) and (7), respectively. As the system size grows larger, and as the mass ratio m_α/m_β becomes farther from unity, the integrands of (4) and (7) vary more rapid;

hence we should use finer intervals on numerical integration. For all the following data of J and $\{T_i\}$ we checked that decreasing the intervals of integration by a factor 5 did not make significant changes of the results.

From the numerical calculation, we found that the total energy current J decreases with oscillation as the generation n increases (see figure 1). The decrease of J for the generation n shows power law behaviour $J \sim n^{-a}$; the exponent is $a \sim 1$ for sufficiently large m_α (e.g., $a = 1.03$ when $m_\alpha = 3.0$). This result indicates that it is appropriate to discuss the heat current in terms of the generation n rather than the system size N . We note that the system size dependence $J \sim n^{-a} \sim (\ln N)^{-a}$ is the remarkable difference from the behaviour $J \sim N^{-b}$ of periodic or disordered systems.

In order to discuss the contribution of eigenstates of the chain to the total heat current we calculate, as done in [11], cumulative heat current:

$$J_c(\omega) = \Delta T \int_0^\omega \frac{d\omega'}{\pi} \frac{2\gamma^2 \omega'^2}{|\det Y|^2}. \quad (11)$$

The cumulative heat current $J_c(\omega)$ is a monotonically increasing function; the increment of $J_c(\omega)$ in a certain ω -region is the contribution of the eigenstates of the ω -region to the total heat current. For the Fibonacci chain, as shown in figure 2, $J_c(\omega)$ consists of many slopes and plateaus. Each slope consists of slopes and plateaus in nested fashion, and the nested structure becomes finer as the generation grows; i.e., $J_c(\omega)$ seems to become the devil's staircase in the infinite-generation limit.

The devil's staircase-like structure of $J_c(\omega)$ is very similar to the integrated density of states (IDOS) of the Fibonacci chain (see figure 2). The plateaus of $J_c(\omega)$ approximately coincide with the plateaus of the IDOS; i.e., the frequencies corresponding to the eigenstates make major contribution to the heat current.

Figure 2 shows that dominant contribution to J comes from the low frequency eigenstates, especially in high generation. We may attribute the high conductivity in the low-frequency region to the extended eigenstates. The high frequency eigenstates are critical, i.e., they show a power-law decay, while the low frequency eigenstates are extended like eigenstates in periodic chains. Correspondingly, the low frequency eigenstates may transport the energy ballistically. The ballistic transport can be seen from the similarity between $J_c(\omega)$ of the Fibonacci chain and $J_c(\omega)$ of a periodic chain in low frequency region (see figure 2). We should note that the low frequency region in which the eigenstates are extended become narrower in the limit of infinite system size. This is because all the eigenstates become critical in the limit of infinite system size, since the continuous part of the spectrum of the Fibonacci chain narrows and becomes singular continuous even in low frequency region [7]. As a consequence, we can conclude that the heat current, unlike that of the periodic chain, vanishes when $N \rightarrow \infty$.

The similarity between $J_c(\omega)$ and IDOS indicates that the generation dependence of J is explained by the spectral properties of the Fibonacci chain. Now, we consider the n -th generation rational approximants, which is a periodic chain whose unit cell is the n -th generation Fibonacci chain. We denote by σ_n the ω^2 -spectrum of the n -th generation rational approximant; σ_n is given as $\{\omega^2; |\text{tr } \mathcal{M}_n| \leq 2\}$. The spectrum σ_n consists of F_n bands; as n increases, the bands are fragmented into pieces and total bandwidth W_n decreases. We note that W_n obeys a power law $W_n \sim n^{-a'}$ and $a' \sim 1$ [7]. Since the frequency region corresponding to the bandgap does not contribute to the heat current, we conclude that the decay of J with increasing n is similar to the decay of W_n ; thus J obeys the power law as W_n does, as shown in figure 1.

Before showing the local temperature $\{T_i\}$, we define Fibonacci sites and Fibonacci blocks, which seem important to discuss the behavior of $\{T_i\}$. On the n -th generation Fibonacci chain, which consists of F_n sites, the Fibonacci site is the F_j -th site with $j = 1, 2, \dots, n-1$ from left or right ends; i.e., the Fibonacci sites are numbered F_j or $F_n - F_j$. We call a region between neighbouring Fibonacci sites the Fibonacci block. Since $F_j \sim \tau^j$, Fibonacci sites are sparsely distributed around the centre of the chain and densely near the ends. If the chain length is normalized to unity, the Fibonacci sites are approximately at τ^{-j} and $1 - \tau^{-j}$. Thus, as the generation increases, the Fibonacci sites distribution becomes denser near the ends but invariant around the centre of the chain. Correspondingly, the size of the Fibonacci blocks around the centre of the chain stays constant in increasing generation.

Now we plot $\{T_i\}$ with Fibonacci sites in figure 3. We can see that the local temperature oscillates strongly along the chain; especially $\{T_i\}$ has significant leaps at the Fibonacci sites. Furthermore, the interior of each Fibonacci blocks have a bilaterally symmetric temperature distribution. The symmetry is a nontrivial result since the whole system with heat baths at both ends is not bilaterally symmetric. We note that some of the Fibonacci blocks have a symmetric mass sequence, but not all the blocks do.

Another major characteristic of $\{T_i\}$ is an oscillatory behavior for increasing generation. We plot in figure 4 the local temperature on the Fibonacci chains of generation $n = 12, 13, 14$ and 15 . There is an obvious similarity between $\{T_i\}$ of $n = 12$ and $n = 14$, and between $\{T_i\}$ of $n = 13$ and $n = 15$; i.e., $\{T_i\}$ oscillates periodically in generation with period two. We checked that the similarity in $\{T_i\}$ of odd- and even-generation chains is maintained throughout the generations from $n = 6$ to $n = 15$, which correspond to the system size from $N = 13$ to $N = 987$. We may check the oscillation quantitatively by comparing the average local temperature of, e.g., the centre Fibonacci block of each chain. The average temperature of the centre Fibonacci block is distributed between 1.558 and 1.589 for odd-generation chains (from $n = 7$ to $n = 15$); between 1.645 and 1.706 for even-generation chains (from $n = 6$ to $n = 14$). The periodic oscillation implies that the local temperature distribution $\{T_i\}$ does not converge to a definite distribution even in the limit of infinite-generation, i.e., in the thermodynamic limit.

It is interesting to note that the mass-weighted amplitude of critical eigenstates also have leaps at the Fibonacci sites as shown in figure 3. Such behaviour is similar to that of the $\{T_i\}$; thus we may expect that the characteristic of the $\{T_i\}$ partly owes to the critical eigenstates. Since we do not observe a critical eigenstate with the symmetry in the Fibonacci block, we may not attribute the cause of the symmetry of $\{T_i\}$ in Fibonacci sites to the properties of a single critical eigenstate.

In summary, we have shown that the Fourier law is invalid for the harmonic Fibonacci chain as for periodic or disordered harmonic chains. The heat current J depends on the system size N as $J \sim (\ln N)^{-1}$; the anomalous dependence is remarkably different from the periodic or disordered case. The N dependence of J is very similar to the N dependence of the total bandwidth of the frequency spectrum. Such similarity is the consequence of the fact that only the lattice vibration with frequency within the frequency-bands can transport the heat over the length of the chain. We have also obtained the local temperature. The local temperature $\{T_i\}$ strongly oscillates and does not show monotonic change. Both $\{T_i\}$ and the mass-weighted amplitude of critical eigenstates have significant leaps at Fibonacci sites; this fact indicates the close relation between $\{T_i\}$ and eigenstates. We have concluded

that $\{T_i\}$ does not converge to a definite form in the limit of infinite system size since $\{T_i\}$ exhibits two different form depending on the parity of the generation.

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Figure captions

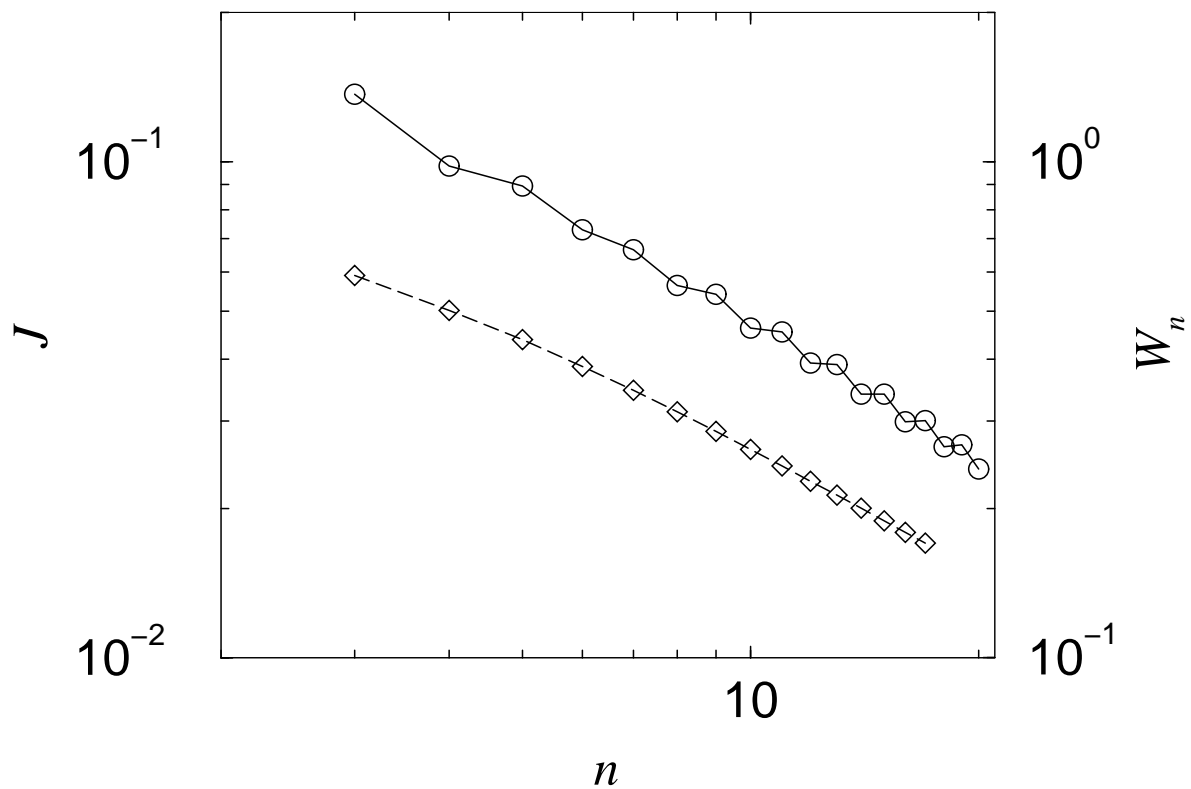


Figure 1. Log-log plot of the generation n versus the heat current J (circle) and the total bandwidth W_n (diamond). Lines are included to guide the eye. The masses of particles in the Fibonacci chain are $m_\alpha = 1.9$ and $m_\beta = 1.0$. The total bandwidth W_n is normalized by the maximum eigenfrequency.

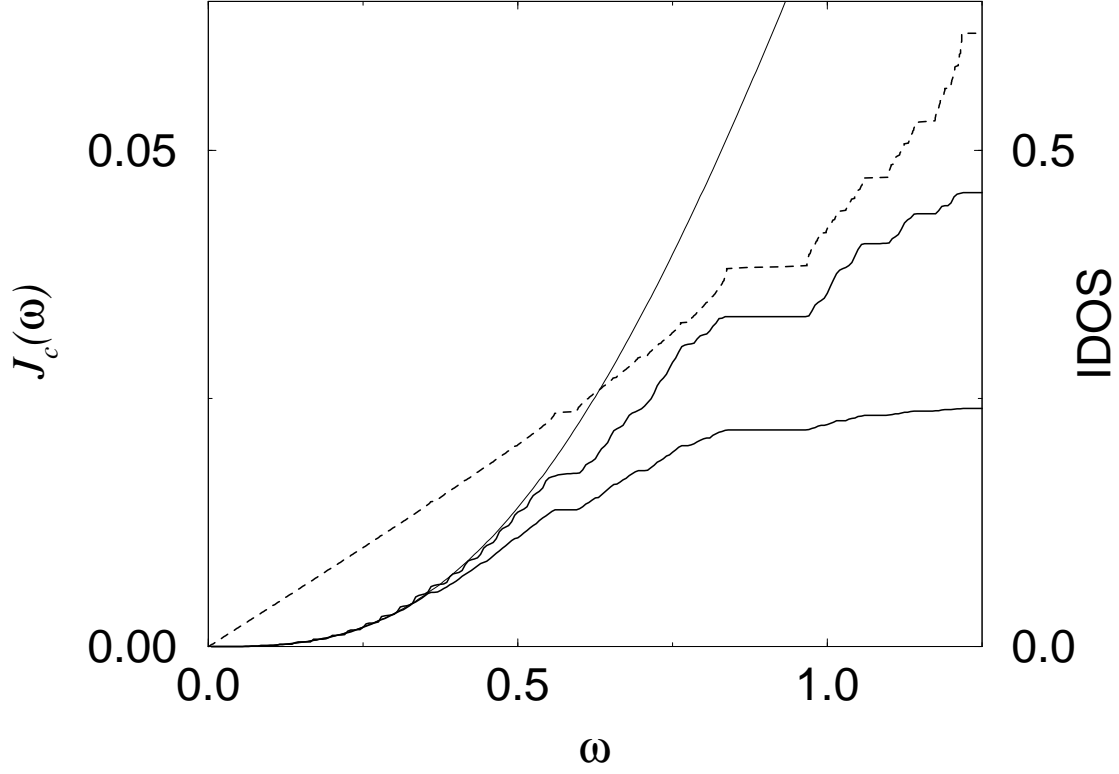


Figure 2. Full lines indicate the cumulative heat currents $J_c(\omega)$. The lower two full lines are $J_c(\omega)$ of 10th (upper line) and 20th (lower line) generation Fibonacci chains with $m_\alpha = 1.9$ and $m_\beta = 1.0$. The upper most smooth full line is $J_c(\omega)$ of a periodic chain with identical particles; the mass of particles is the average of particle in the above two Fibonacci chains. Dashed line is the IDOS of the 15th generation Fibonacci chain. Although there are eigenstates in the high-frequency region (up to $\omega \sim 1.7$), we plot only low- and middle-frequency region because high frequency states contribute little to $J_c(\omega)$.

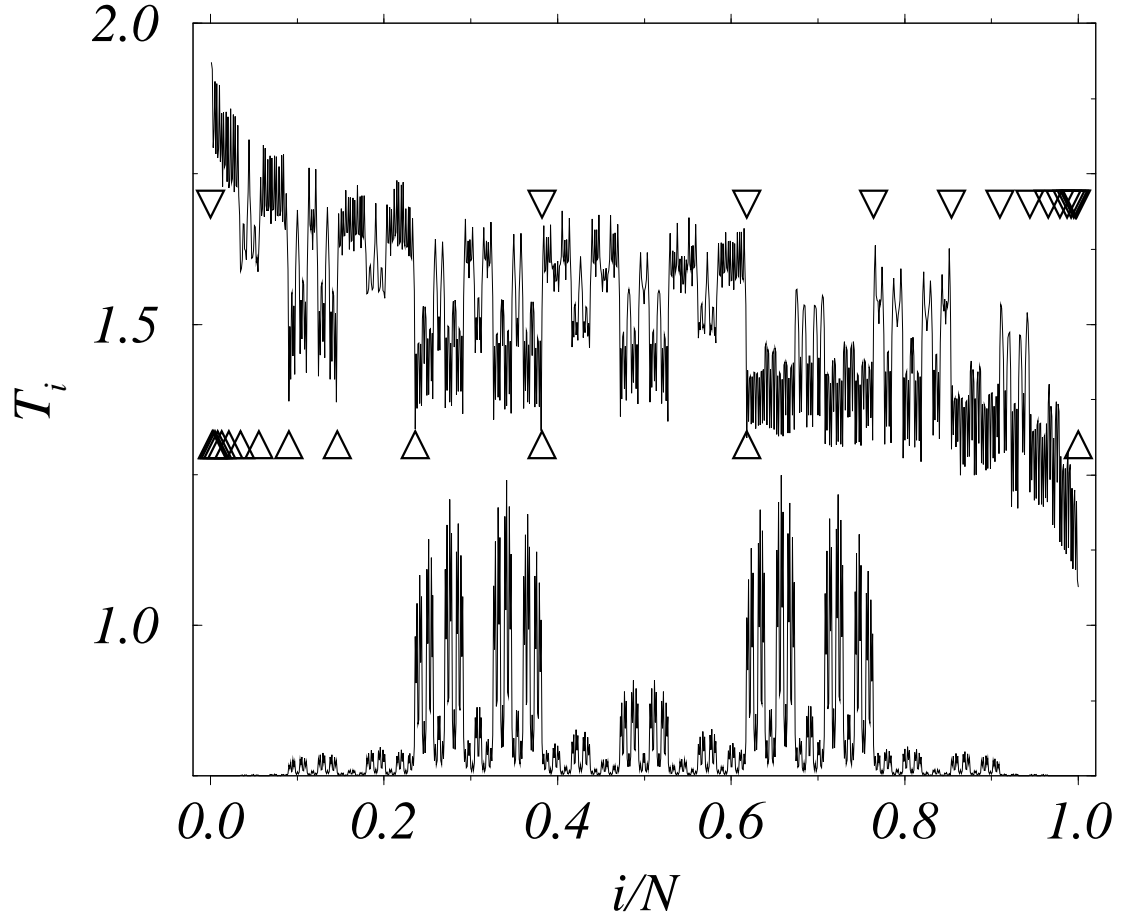


Figure 3. Upper full line is local temperature $\{T_i\}$ on the 15th generation Fibonacci chain with $m_\alpha = 1.9$ and $m_\beta = 1.0$. Triangles indicate the Fibonacci sites: upward and downward triangles correspond to F_j -th and $(F_{15} - F_j)$ -th sites, respectively. Lower full line is $m_i x_i^2(\omega)$ of a critical eigenstate corresponding to the maximum eigenfrequency.

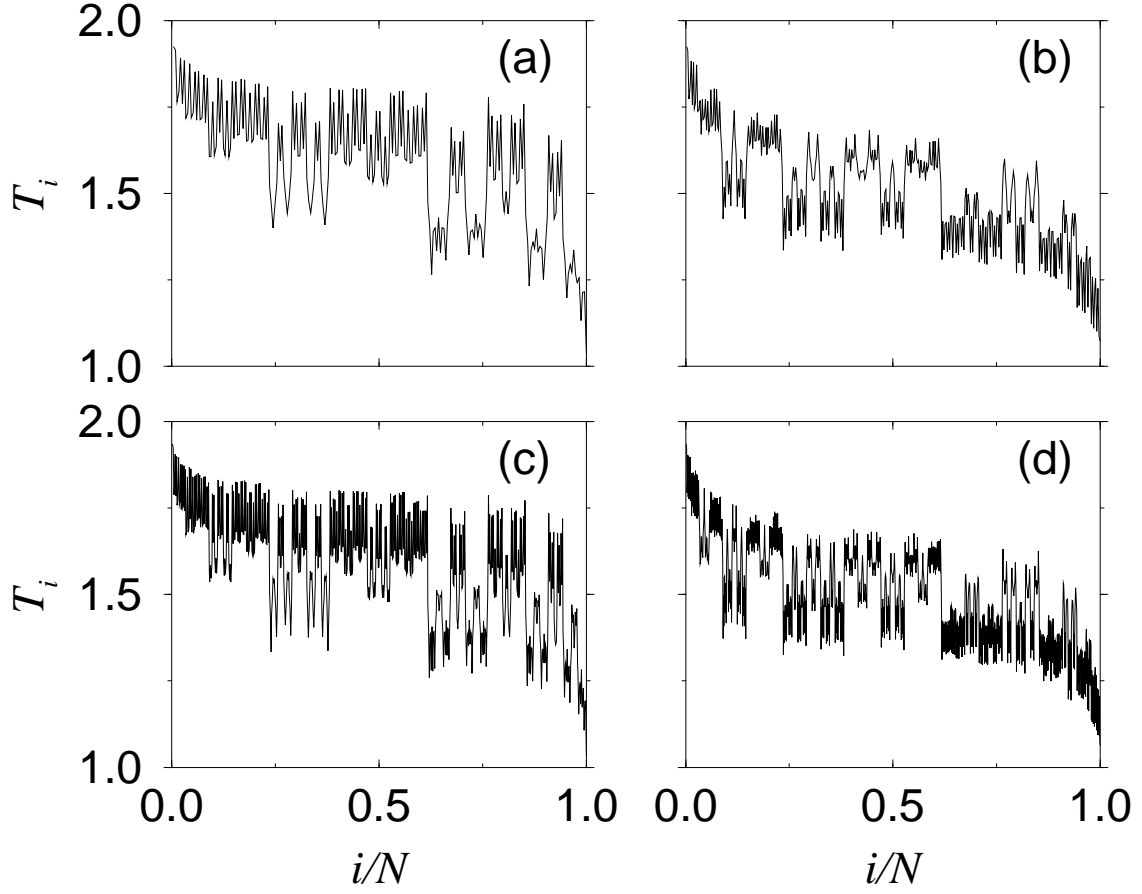


Figure 4. Local temperature on Fibonacci chain of (a) generation $n = 12$ (number of particles $N = 233$), (b) $n = 13$ ($N = 377$), (c) $n = 14$ ($N = 610$), and (d) $n = 15$ ($N = 987$). The Fibonacci chains consist of particles of $m_\alpha = 1.9$ and $m_\beta = 1.0$. Each chain length is normalized to unity.